1,3-Benzenedicarboxylic acid

Other names:	Acide isophtalique
	Benzene,1,3-dicarboxylic acid
	IPA
	Kyselina isoftalova
	NSC 15310
	isophthalic acid
	m-benzenedicarboxylic acid
	m-dicarboxybenzene
	m-phthalic acid
Inchi:	InChI=1S/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)(H,11,12)
InchiKey:	QQVIHTHCMHWDBS-UHFFFAOYSA-N
Formula:	C8H6O4
SMILES:	O=C(O)c1cccc(C(=O)O)c1
Mol. weight [g/mol]:	166.13
CAS:	121-91-5

Physical Properties

Property code	Value	Unit	Source
af	0.8464		Cheméo Relay (1.0)
chs	-3204.10 ± 1.50	kJ/mol	NIST Webbook
chs	-3215.37	kJ/mol	NIST Webbook
chs	-3217.85	kJ/mol	NIST Webbook
chs	-3202.60 ± 0.50	kJ/mol	NIST Webbook
gf	-412.22	kJ/mol	Joback Method
hf	-647.09	kJ/mol	Cheméo Relay (1.0)
hfs	-803.04	kJ/mol	NIST Webbook
hfs	-801.50 ± 1.50	kJ/mol	NIST Webbook
hfus	21.50	kJ/mol	Joback Method
hsub	142.00 ± 0.70	kJ/mol	NIST Webbook
hvap	112.25	kJ/mol	Cheméo Relay (1.0)
ie	10.00 ± 0.20	eV	NIST Webbook
log10ws	-1.83		Cheméo Relay (1.0)
logp	1.083		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
tb	559.17	K	Cheméo Relay (1.0)
tc	852.88	K	Cheméo Relay (1.0)

tf	621.20	K	Solid-Liquid Equilibria for Benzoic Acid + p-Toluic Acid + Chloroform, Benzoic Acid + p-Toluic Acid + Acetic Acid, and Terephthalic Acid + Isophthalic Acid + N,N-Dimethylformamide
vc	0.409	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.80	J/mol×K	706.20	Joback Method
cpg	289.37	J/mol×K	739.78	Joback Method
cpg	295.47	J/mol×K	773.36	Joback Method
cpg	301.12	J/mol×K	806.93	Joback Method
cpg	306.34	J/mol×K	840.51	Joback Method
cpg	311.15	J/mol×K	874.09	Joback Method
cpg	315.57	J/mol×K	907.67	Joback Method
cps	201.70	J/mol×K	323.00	NIST Webbook
cps	201.70	J/mol×K	323.00	NIST Webbook
dvisc	0.0004918	Pa×s	484.67	Joback Method
dvisc	0.0002081	Pa×s	528.97	Joback Method
dvisc	0.0001006	Pa×s	573.28	Joback Method
dvisc	0.0000539	Pa×s	617.59	Joback Method
dvisc	0.0000314	Pa×s	661.89	Joback Method
dvisc	0.0000196	Pa×s	706.20	Joback Method
dvisc	0.0013822	Pa×s	440.36	Joback Method
hfust	43.20	kJ/mol	617.40	NIST Webbook
hsubt	134.60 ± 1.60	kJ/mol	450.00	NIST Webbook
hsubt	114.20	kJ/mol	528.00	NIST Webbook
hsubt	106.70 ± 2.20	kJ/mol	528.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.32607e+02

Coeff. B	-2.87138e+04
Coeff. C	-2.91467e+01
Coeff. D	5.64805e-06
Temperature range (K), min.	619.15
Temperature range (K), max.	1007.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=968

Solubilities of 1,3,5-Benzenetricarboxylic Acid and 1,3-Benzenedicarboxylic Acid in Acetic Acid + Water Solvent Mixtures: https://www.doi.org/10.1021/je800353s

Chemeo Relay (1.0):

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Understanding the enhanced solubility of 1,3-benzenedicarboxylic acid in polar binary solvents of (acetone + water) at various temperatures: https://www.doi.org/10.1016/j.jct.2016.10.011

Solubilities of 1,3-benzenedicarboxylic acid in Water + Acetic Acid Solutions: https://www.doi.org/10.1021/je049784c

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Solid-Liquid Equilibria for Benzoic Acid + p-Toluic Acid + Chloroform, Benzoic Acid + p-Toluic Acid + Acetic Acid, and Terephthalic Acid + Isophthalic Acid + N,N-Dimethylformamide: https://www.doi.org/10.1021/je049801y

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Determination and prediction of solid-liquid phase equilibrium for quaternary system of terephthalic acid + isophthalic acid + phthalic acid + N-methyl-2-pyrrolidone at 303.15 K and 313.15 K: https://www.doi.org/10.1016/j.fluid.2015.03.042

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Phase Equilibrium and Phase Diagram for the System of Benzene Dicarboxylic Acid + N-Methyl-2-pyrrolidone: https://www.doi.org/10.1021/je500542j

Chemeo Relay (120, beta):

Solubilities of Benzene Carboxylic Acids in Isobutyl Acetate from (299.73 to 353.15) K: https://www.doi.org/10.1021/je101319f

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121915&Units=SI

Measurements of the solubilties of m-phthalic acid in acetone, ethanol and acetic ether: https://www.doi.org/10.1016/j.fluid.2008.01.014

Solubilities of Terephthalic Acid, Phthalic Acid, and Isophthalic Acid in Tetrahydrofuran, Cyclohexanone, 1,2-Diethoxyethane, and Acetophenone: https://www.doi.org/10.1021/je9001976

Measurement and Correlation of the Solubilities of m-Phthalic Acid in Monohydric Alcohols: https://www.doi.org/10.1021/je800520w

Solubilities of Isophthalic Acid in Ternary Mixtures of Acetic Acid + Water + Benzoic Acid from 292.55 to 372.10 K: https://www.doi.org/10.1021/acs.jced.7b00958

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume